

Combined effect of nonmagnetic and magnetic scatterers on critical temperatures of superconductors with different gap anisotropy

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The combined effect of nonmagnetic and magnetic defects and impurities on critical temperatures of superconductors with different gap anisotropy is studied theoretically within the weak coupling limit of the BCS model. An expression is derived which relates the critical temperature to relaxation rates of charge carriers by nonmagnetic and magnetic scatterers, as well as to the coefficient of anisotropy of the superconducting order parameter on the Fermi surface. Particular cases of d -wave, $(s + d)$ -wave, and anisotropic s -wave superconductors are briefly discussed.

This paper is motivated by conflicting experimental results concerning the symmetry of the superconducting order parameter $\Delta(\mathbf{p})$ in high-temperature superconductors (HTSCs) and the suppression of the critical temperature T_c of HTSCs by defects and impurities. Indeed, while the majority (though not all) of experiments support the d -wave superconductivity in HTSCs [1], the observed degradation of T_c by impurities or radiation-induced defects [2] is more gradual than predicted theoretically for d -wave superconductors [3].

To resolve this contradiction, a number of suggestions have been made, including anisotropic s -wave symmetry of $\Delta(\mathbf{p})$ [4], momentum dependence of impurity scattering [5], strong coupling effects resulting in crossover from Cooper pairs to local bosons [6], *etc.* Note, however, that theoretical analysis of T_c degradation by defects and impurities is usually restricted to the specific case of spin-independent scattering potential, i.e., to the case of nonmagnetic scatterers only. Meanwhile a lot of experiments give evidence for the presence of magnetic scatterers (along with nonmagnetic ones) in non-stoichiometric HTSCs, e.g., in oxygen-deficient, doped or irradiated samples [7].

The goal of this paper is to work out a theoretical framework for a description of *combined* effect of nonmagnetic and magnetic scatterers on T_c of a superconductor with anisotropic $\Delta(\mathbf{p})$ (in what concerns an isotropic s -wave superconductor, its T_c is insensitive to nonmagnetic defects [8], while the T_c suppression by magnetic defects is given by a well-known Abrikosov-Gor'kov theory [9]). We use the weak coupling limit of the BCS model for superconducting pairing and the Born approximation for impurity scattering. In what follows, we do not specify the microscopic mechanism of superconductivity. We set $\hbar = k_B = 1$ throughout the paper.

The Hamiltonian of a superconductor containing both nonmagnetic and magnetic scatterers reads

$$\hat{H} = \sum_{\mathbf{p}, \sigma} \xi(\mathbf{p}) \hat{a}_{\mathbf{p}\sigma}^+ \hat{a}_{\mathbf{p}\sigma} + \sum_{\mathbf{p}, \mathbf{p}', \sigma, \sigma'} U(\mathbf{p}, \sigma; \mathbf{p}', \sigma') \hat{a}_{\mathbf{p}\sigma}^+ \hat{a}_{\mathbf{p}'\sigma'} + \sum_{\mathbf{p}, \mathbf{p}'} V(\mathbf{p}, \mathbf{p}') \hat{a}_{\mathbf{p}\uparrow}^+ \hat{a}_{-\mathbf{p}\downarrow}^+ \hat{a}_{-\mathbf{p}'\downarrow} \hat{a}_{\mathbf{p}'\uparrow}, \quad (1)$$

where $\xi(\mathbf{p}) = \epsilon(\mathbf{p}) - \mu$ is the quasiparticle energy measured from the chemical potential, $U(\mathbf{p}, \sigma; \mathbf{p}', \sigma')$ is the matrix element for electron scattering by randomly distributed impurities (defects) from the state (\mathbf{p}', σ') to the state (\mathbf{p}, σ) , and $V(\mathbf{p}, \mathbf{p}')$ is the BCS pair potential.

We assume for simplicity that electron scattering is isotropic in the momentum space, the amplitude of the scattering by an isolated nonmagnetic (magnetic) scatterer being u_n (u_m). Then the relaxation times τ_n and τ_m are given by the standard "golden rule" formulas

$$\frac{1}{\tau_n} = 2\pi c_n |u_n|^2 N(0), \quad \frac{1}{\tau_m} = 2\pi c_m |u_m|^2 N(0), \quad (2)$$

where c_n and c_m are the concentrations of scatterers, $N(0)$ is the density of electron states at the Fermi level. Note that the commonly accepted expression for $|u_m|^2$ is $J^2 S(S+1)/4$, where J is the energy of electron-impurity exchange interaction, S is the impurity spin.

In order to account for anisotropy of the superconducting state, we assume a factorizable pairing interaction of the form [10]

$$V(\mathbf{p}, \mathbf{p}') = -V_0 \phi(\mathbf{n}) \phi(\mathbf{n}'), \quad (3)$$

where $\mathbf{n} = \mathbf{p}/p$ is a unit vector along the momentum. Then the order parameter $\Delta(\mathbf{p})$ is [10]

$$\Delta(\mathbf{p}) = \Delta_0 \phi(\mathbf{n}), \quad (4)$$

where Δ_0 depends on the temperature. Thus the function $\phi(\mathbf{n})$ specifies the anisotropy of $\Delta(\mathbf{p})$ in the momentum space ($\phi(\mathbf{n}) \equiv 1$ for isotropic pairing). The self-consistent equation for $\Delta(\mathbf{p})$ can be derived by means of Green's functions technique (see, e.g., [9]). It is as follows:

$$\Delta(\mathbf{p}) = - \sum_{\mathbf{p}'} V(\mathbf{p}, \mathbf{p}') \langle \hat{a}_{-\mathbf{p}'\downarrow} \hat{a}_{\mathbf{p}'\uparrow} \rangle = -T \sum_{\omega} \sum_{\mathbf{p}'} V(\mathbf{p}, \mathbf{p}') \frac{\Delta_{\omega}(\mathbf{p}')}{\omega'^2 + \xi^2(\mathbf{p}') + |\Delta_{\omega}(\mathbf{p}')|^2}, \quad (5)$$

where $\omega = \pi T(2n + 1)$ are Matsubara frequencies, and the equations for $\Delta_{\omega}(\mathbf{p})$ and ω' are

$$\Delta_{\omega}(\mathbf{p}) = \Delta(\mathbf{p}) + (c_n |u_n|^2 - c_m |u_m|^2) \sum_{\mathbf{p}'} \frac{\Delta_{\omega}(\mathbf{p}')}{\omega'^2 + \xi^2(\mathbf{p}') + |\Delta_{\omega}(\mathbf{p}')|^2}, \quad (6)$$

$$\omega' = \omega - i(c_n |u_n|^2 + c_m |u_m|^2) \sum_{\mathbf{p}'} \frac{i\omega' + \xi(\mathbf{p}')}{\omega'^2 + \xi^2(\mathbf{p}') + |\Delta_{\omega}(\mathbf{p}')|^2}. \quad (7)$$

Since $\Delta(\mathbf{p}) = 0$ at $T = T_c$, in the case $T \rightarrow T_c$ we have from (6), (7), taking (2) into account:

$$\Delta_{\omega}(\mathbf{p}) = \Delta(\mathbf{p}) + \frac{1}{2|\omega'|} (1/\tau_n - 1/\tau_m) \langle \Delta_{\omega}(\mathbf{p}) \rangle, \quad (8)$$

$$\omega' = \omega + \frac{1}{2} (1/\tau_n + 1/\tau_m) \text{sign}(\omega), \quad (9)$$

where angular brackets $\langle \dots \rangle$ stand for the average over the Fermi surface (FS):

$$\langle \dots \rangle = \int_{FS} (\dots) \frac{d\Omega_{\mathbf{p}}}{|\partial \xi(\mathbf{p})/\partial \mathbf{p}|} \bigg/ \int_{FS} \frac{d\Omega_{\mathbf{p}}}{|\partial \xi(\mathbf{p})/\partial \mathbf{p}|}. \quad (10)$$

Substituting (8) and (9) in (5) and taking (3) into account, we have after rather simple but time consuming algebraic transformations:

$$\ln \left(\frac{T_{c0}}{T_c} \right) = \pi T_c \sum_{\omega} \frac{1}{|\omega| + \frac{1}{2} (1/\tau_n + 1/\tau_m)} \left[\frac{1}{2|\omega|} (1/\tau_n + 1/\tau_m) - \frac{\langle \phi(\mathbf{n}) \rangle^2}{\langle \phi^2(\mathbf{n}) \rangle} \cdot \frac{1/\tau_n - 1/\tau_m}{2(|\omega| + 1/\tau_m)} \right]. \quad (11)$$

Here T_{c0} is the critical temperature in the absence of impurities and defects (at $1/\tau_n = 1/\tau_m = 0$). At this stage it is convenient to introduce the coefficient χ of anisotropy of the order parameter on the FS [10], [4]

$$\chi = 1 - \frac{\langle \phi(\mathbf{n}) \rangle^2}{\langle \phi^2(\mathbf{n}) \rangle} = 1 - \frac{\langle \Delta(\mathbf{p}) \rangle^2}{\langle \Delta^2(\mathbf{p}) \rangle}. \quad (12)$$

For isotropic s -wave pairing we have $\Delta(\mathbf{p}) \equiv \text{const}$ on the FS; therefore, $\langle \Delta(\mathbf{p}) \rangle^2 = \langle \Delta^2(\mathbf{p}) \rangle$, and $\chi = 0$. For a superconductor with d -wave pairing we have $\chi = 1$ since $\langle \Delta(\mathbf{p}) \rangle = 0$. The range $0 < \chi < 1$ corresponds to anisotropic s -wave pairing or to mixed ($d + s$)-wave pairing. The higher is the anisotropy of $\Delta(\mathbf{p})$ (e.g., the greater is the partial weight of a d -wave in the case of mixed pairing), the closer to unity is the value of χ .

Making use of the definition (12) and the formula [11]

$$\sum_{k=0}^{\infty} \left(\frac{1}{k+x} - \frac{1}{k+y} \right) = \Psi(y) - \Psi(x), \quad (13)$$

where Ψ is the digamma function, we obtain from (11):

$$\ln \left(\frac{T_{c0}}{T_c} \right) = (1 - \chi) \left[\Psi \left(\frac{1}{2} + \frac{1}{2\pi T_c \tau_m} \right) - \Psi \left(\frac{1}{2} \right) \right] + \chi \left[\Psi \left(\frac{1}{2} + \frac{1}{4\pi T_c} \cdot \left(\frac{1}{\tau_n} + \frac{1}{\tau_m} \right) \right) - \Psi \left(\frac{1}{2} \right) \right]. \quad (14)$$

In two particular cases of (i) both nonmagnetic and magnetic scattering in an isotropic s -wave superconductor ($\chi = 0$) and (ii) nonmagnetic scattering only in a superconductor with arbitrary anisotropy of $\Delta(\mathbf{p})$ ($1/\tau_m = 0$, $0 \leq \chi \leq 1$), the Eq.(14) reduces to well-known expressions [9], [10]

$$\ln \left(\frac{T_{c0}}{T_c} \right) = \Psi \left(\frac{1}{2} + \frac{1}{2\pi T_c \tau_m} \right) - \Psi \left(\frac{1}{2} \right) \quad (15)$$

and

$$\ln \left(\frac{T_{c0}}{T_c} \right) = \chi \left[\Psi \left(\frac{1}{2} + \frac{1}{4\pi T_c \tau_n} \right) - \Psi \left(\frac{1}{2} \right) \right]. \quad (16)$$

respectively.

The Eq. (14) is obviously more general than Eqs.(15) and (16) which are commonly used for the analysis of experimental data on T_c suppression by defects and impurities in HTSCs [12]. In fact, making use of Eq. (15) or Eq.(16) one *assumes a priori* that either (i) the order parameter in HTSCs is isotropic in the momentum space or (ii) the magnetic scatterers in HTSCs are completely absent. The latter assumption is often supplemented with a speculation about pure d -wave symmetry of $\Delta(\mathbf{p})$ [13] (i.e., one intentionally restricts himself to the case $\chi = 1$ instead of attempts to extract the value of χ from the experiment). In our opinion, the experimental dependencies of T_c versus impurity (defect) concentration or radiation dose should be analyzed within the framework of the theory presented above, see Eq.(14). One should not *guess* as to the degree of anisotropy of $\Delta(\mathbf{p})$ and the type of scatterers, but try to *determine* the value of χ and relative weights of magnetic and nonmagnetic components in electron scattering through comparison of theoretical predictions with available or specially performed experiments.

Now let us consider the limiting cases of weak and strong scattering ($T_{c0} - T_c \ll T_{c0}$ and $T_c \rightarrow 0$ respectively). At $1/4\pi T_{c0} \tau_n \ll 1$ and $1/4\pi T_{c0} \tau_m \ll 1$ (weak scattering) one has from (14):

$$T_{c0} - T_c \approx \frac{\pi}{4} \left[\frac{\chi}{2\tau_n} + \frac{1 - \chi/2}{\tau_m} \right]. \quad (17)$$

In particular cases (i) and (ii) considered above, Eq.(17) reduces to well-known expressions [12]

$$T_{c0} - T_c \approx \frac{\pi}{4\tau_m} \quad (18)$$

and

$$T_{c0} - T_c \approx \frac{\pi\chi}{8\tau_n} \quad (19)$$

for initial T_c reduction by magnetic (at $\chi = 0$) or nonmagnetic (at arbitrary value of χ) scatterers respectively.

In what concerns the strong scattering limit, we recall that in the BCS theory, nonmagnetic scattering alone is insufficient for the not- d -wave superconductivity ($0 \leq \chi < 1$) to be destroyed completely [10]; at $1/\tau_m = 0$, the value of T_c asymptotically goes to zero as $1/\tau_n$ increases (whereas T_c of a d -wave superconductor with $\chi = 1$ vanishes at a critical value $1/\tau_n^c = \pi T_{c0}/\gamma \approx 1.764 T_{c0}$, where $\gamma = e^C \approx 1.781$, C is the Euler constant). On the other hand, magnetic scattering in the absence of nonmagnetic one ($1/\tau_n = 0$) is known to suppress the isotropic s -wave superconductivity with $\chi = 0$ at a critical value $1/\tau_m^c = \pi T_{c0}/2\gamma \approx 0.882 T_{c0}$ [9].

Based on the Eq.(14), it is straightforward to derive the general condition for impurity (defect) suppression of T_c of a superconductor having an arbitrary anisotropy coefficient χ and containing both nonmagnetic and magnetic scatterers:

$$\frac{1}{\tau_{eff}^c} = \frac{\pi}{\gamma} 2^{\chi-1} T_{c0}, \quad (20)$$

where τ_{eff}^c is the critical value of the effective relaxation time τ_{eff} defined as

$$\frac{1}{\tau_{eff}} = \left(\frac{1}{\tau_m} \right)^{1-\chi} \cdot \left(\frac{1}{\tau_n} + \frac{1}{\tau_m} \right)^\chi. \quad (21)$$

From Eqs. (20) and (21) one can see that $1/\tau_{eff}^c$ increases monotonically with both $1/\tau_n$ and $1/\tau_m$ at any value of χ , with the exception of the case $\chi = 0$ when $1/\tau_{eff}^c$ doesn't depend on $1/\tau_n$, see (21). If χ is close to unity (strongly

anisotropic $\Delta(\mathbf{p})$), then $1/\tau_{eff} \approx 1/\tau_n + 1/\tau_m$, i.e., the contribution of nonmagnetic and magnetic scattering to pair breaking is about the same. If $\chi \ll 1$ (almost isotropic $\Delta(\mathbf{p})$), then $1/\tau_{eff} \approx 1/\tau_m$, i.e., τ_{eff} is determined primarily by magnetic scattering. The higher is the anisotropy coefficient χ , the greater is the relative contribution of nonmagnetic scatterers to T_c degradation with respect to magnetic ones. If nonmagnetic scattering is absent ($1/\tau_n = 0$), then $1/\tau_{eff} = 1/\tau_m$ at any value of χ .

We note however that while the concept of the effective relaxation time τ_{eff} can be used for evaluation of the *critical* level of nonmagnetic and magnetic disorder, it is not possible to express T_c in terms of τ_{eff} in the *whole range* $0 \leq T_c \leq T_{c0}$, see (14). In other words, the combined effect of nonmagnetic and magnetic scattering on T_c cannot be described by a single universal parameter depending on the values of τ_n , τ_m , and χ . For example, $1/\tau_{eff} = 0$ at $1/\tau_m = 0$ and $0 \leq \chi < 1$ no matter what the value of $1/\tau_n$ is. On the one hand, as follows from (20), the zero value of $1/\tau_{eff}^c$ in this case points to the fact that in a BCS superconductor with not-*d*-wave symmetry of $\Delta(\mathbf{p})$ the critical level of disorder cannot be reached in the absence of magnetic scattering, in accordance with [10]. On the other hand, the zero value of $1/\tau_{eff}$ obviously doesn't imply that T_c of a not-*d*-wave superconductor is completely insensitive to nonmagnetic scatterers at $1/\tau_m = 0$ and $0 < \chi < 1$, see (14). Hence, while the quantity $1/\tau_{eff}^c$ characterizes the critical strength of impurity (defect) scattering corresponding to $T_c = 0$, the quantity $1/\tau_{eff}$ (when it is less than $1/\tau_{eff}^c$) doesn't determine the value of T_c unequivocally.

Based on Eqs. (20) and (21), it is possible to derive the following expression for the critical value of $1/\tau_n$ in the presence of magnetic scattering:

$$\frac{1}{\tau_n^c} = \frac{1}{\tau_m} \left[2 \left(\frac{\pi T_{c0} \tau_m}{2\gamma} \right)^{1/\chi} - 1 \right]. \quad (22)$$

This expression is valid as long as $1/\tau_m < \pi 2^{\chi-1} T_{c0}/\gamma$ since otherwise the superconductivity is completely suppressed solely by magnetic impurities. The value of $1/\tau_n^c$ decreases as $1/\tau_m$ increases at constant χ or as χ increases at constant $1/\tau_m$. The finite value of $1/\tau_n^c$ in the presence of magnetic scatterers could reconcile the experimentally observed disorder-induced suppression of T_c of HTSCs below 4.2K [2] with theories of not purely *d*-wave symmetry of $\Delta(\mathbf{p})$ in HTSCs, e.g., anisotropic *s*-wave symmetry or mixed (*d* + *s*)-wave symmetry.

In conclusion, the results obtained provide the basis for evaluation of the degree of anisotropy of the superconducting order parameter (and hence its possible symmetry) as well as the type of scatterers (magnetic or nonmagnetic) in high- T_c superconductors through careful comparison of theoretical predictions with the experiments on impurity-induced and radiation-induced reduction of the critical temperature. We hope that the present paper will serve as a stimulus for experiments on combined effect of nonmagnetic and magnetic scattering in the copper-oxide superconductors.

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